

# MOLECULAR DYNAMICS SIMULATIONS OF THE ELASTIC MODULUS OF POLYMER-CARBON NANOTUBE COMPOSITES

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The elastic modulus of polymer-carbon nanotube composites is investigated by molecular dynamics simulations of a single-walled carbon nanotube embedded in polyethylen. As a fully hydrocarbon system, we represent the polyethylene matrix with either a many-bond order potential based on Brenner or a united-atom potential. To derive stress-strain curves we use the Parrinello-Rahman approach to apply external stress to a periodic system. To compare the stress-strain curves with rule-of-mixtures predictions three periodic systems, an infinite carbon nanotube, a finite carbon nanotube embedded in polyethylene and the polyethylene matrix itself, are investigated. Furthermore the influence of the nanotube/polyethylene ratio on the elastic modulus is examined. The results show an excellent agreement with the rule-of-mixtures.

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